# First-Principles Calculations of Hydrogen Vibrations in Metal Hydrides

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**Abstract**

With recent developments in first-principles electronic-structure calculations, it has become possible to accurately evaluate the vibrational modes in solids. These vibrational modes have become a powerful means to study hydrogen characteristics in metal hydrides, which are technologically important materials in the energy industry. We have applied the state-of-the-art computational techniques to investigate hydrogen vibrations in various metal hydrides. These vibrational modes provide valuable information on the potential energy surface of hydrogen in the host. I will discuss a few examples in transition metal hydrides and make connection with more complex hydrides of current interest.